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Microscopic collective dynamics of atoms in the amorphous metallic alloy Ni33Zr67

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Abstract

The structural properties and microscopic collective dynamics of atoms in the amorphous metallic alloy Ni33Zr67 are studied using molecular dynamics simulations with a pair-additive model potential. The calculated equilibrium structural and dynamic characteristics are compared with experimental data on neutron diffraction and inelastic X-ray scattering. Theoretical analysis of the structural relaxation of microscopic density fluctuations for amorphous metallic alloys is performed within the Lee's recurrent relation approach. The results of theoretical calculations for the intensity of scattering I(k, ω) for the amorphous metallic alloy Ni33Zr67 are in good agreement with the results of computer simulation and experimental inelastic X-ray scattering data. The low-frequency excitations observed in the longitudinal current spectra are related to the vibrational motions of individual atom clusters, which include Ni and Zr atoms. © 2014 Pleiades Publishing, Ltd.

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